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DIRECT NONPERIODIC AND PERIODIC CUBIC SPLINES

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This paper deals with two direct cubic splines, one nonperiodic (up to initial conditions), and one periodic (up to boundary conditions) which both fit the second derivatives of a function at mesh points.

1. Introduction. Cubic splines were first introduced by Schoenberg [5] to fit equally spaced data by analytic functions. Since then many authors have contributed to the theory of splines. The genesis and characterization of cubic (and other) splines are described in detail in Ahlberg et al. [1] and De Boor [2].

In a recent paper El Tarazi and Sallam [3] have constructed a quartic spline which interpolates the first derivatives of a given function at the knots and the second derivatives between them.

In this paper two different direct cubic splines are considered that interpolate the second derivatives of a function at the knots. The first, called nonperiodic, satisfies initial conditions. The second, called periodic, satisfies periodic boundary conditions.

Sections 2 and 3 contain the construction and the existence and uniqueness study of the direct nonperiodic cubic spline. Error bounds for the function and its first three derivatives are derived. In Sections 4 and 5 the direct periodic cubic spline with similar error bounds is presented and finally in Section 6 several numerical examples are given showing, together with the theoretical error bounds on the function and its first three derivatives, the proposed splines to be efficient.

2. The Nonperiodic Case (Existence and Uniqueness). Let $\{x_i,\ i=0,1,\dots,N\}$ be a uniform partition of $[0,1]$. Denote by $S^2_{N,3}$ the linear space of cubic splines $s(x)$ such that

$s(x)\in C^2[0,1]$;

$s(x)$ is a cubic polynomial in each subinterval $[x_i, x_{i+1}]$. Set $h=x_{i+1}-x_i$ $(i=0,1,\dots,N-1)$. If g is a real-valued function defined in $[0,1]$, then g_i is $g(x_i)$ $(i=0,1,\dots,N)$.

Theorem 1. *Given the real numbers f''_i $(i=0,1,\dots,N)$, f_0 and f'_0, there exists a unique $s\in S^{(2)}_{N,3}$ such that*

$$s''_i=f''_i\ (i=0,1,\dots,N),\qquad s_0=f_0,\ s'_0=f'_0, \tag{2.1}$$

where primes denote differentiation with respect to x. The cubic spline satisfying (2.1) in $[x_i, x_{i+1}]$ is

$$s(x)=s_iA_0(t)+hs'_iA_1(t)+h^2f''_iA_2(t)+h^2f''_{i+1}A_3(t), \tag{2.2}$$

where

(2.3) $$A_0(t)=1,\quad A_1(t)=t,\quad A_2(t)=\frac{1}{2}t^2-\frac{1}{6}t^3,\quad A_3(t)=\frac{1}{6}t^3$$

and $t=(x-x_i)/h$.

The coefficients s_i and s'_i in (2.2) are given by the recurrence formulae:

(2.4) $$\begin{aligned} s'_i&=s'_{i-1}+\frac{h}{2}(f''_{i-1}+f''_i),\\ s_i&=s_{i-1}+h\,s'_{i-1}+\frac{h^2}{6}(2f''_{i-1}+f''_i),\\ s_0&=f_0,\quad s'_0=f'_0,\quad (i=1,2,\dots,N). \end{aligned}$$

Proof. If $P_3(t)$ is a cubic polynomial in $[0,1]$, then it can be written as

$$P_3(t)=P_3(0)A_0(t)+P'_3(0)A_1(t)+P''_3(0)A_2(t)+P''_3(1)A_3(t).$$

To determine A_0, A_1, A_2 and A_3 we write the equality for $P_3(t)\equiv 1$, t, t^2 and t^3. We obtain the linear system

$$\begin{aligned} 1&=A_0(t)\\ t&=A_1(t)\\ t^2&=2A_2(t)+2A_3(t)\\ t^3&=6A_3(t) \end{aligned}$$

from which it follows that

$$A_0(t)=1,\quad A_1(t)=t,\quad A_2(t)=\frac{t^2}{3}-\frac{t^3}{6},\quad A_3(t)=\frac{t^3}{6}.$$

Now for a fixed $i\in\{0,1,\dots,N-1\}$, set $x=x_i+$th, $0\leq t\leq 1$. In $[x_i, x_{i+1}]$ the cubic spline $s(x)$ which satisfies (2.1) is

$$s(x)=s_iA_0(t)+hs'_iA_1(t)+h^2f''_iA_2(t)+h^2f''_{i+1}A_3(t).$$

A similar expression holds for $s(x)$ in $[x_{i-1}, x_i]$. Since $s(x)\in C^2[0,1]$, so the continuity conditions $s(x_i^-)=s(x_i^+)$ and $s'(x_i^-)=s'(x_i^+)$ lead to the above recurrence formulae (2.4). [For i=N (2.4) is directly satisfied by (2.2) and (2.3)]. This completes the proof.

3. Error Estimates for the Nonperiodic Case. In this section L_∞ error estimates re given for the above interpolating cubic spline and its first three derivatives in 0,1]. $\|\cdot\|$ denotes the L_∞ norm.

Lemma 1. *Let* s(x) *be the cubic spline defined in* (2.2) *and* (2.4). *If* $f\in C^4[0,1]$ hen $(i=0,1,\dots,n)$

(3.1) $$|s'_i-f'_i|\leq\frac{h^2}{12}\|f^{(4)}\|$$

Proof. We have from (2.4)

$$s'_i=s'_0+\frac{h}{2}(f''_0+f''_i+2\sum_{j=1}^{i-1}f''_j).$$

Thus

(3.2) $$s'_i-f'_i=s'_0-f'_0+\frac{h}{2}(f''_0+f''_i+2\sum_{j=1}^{i-1}f''_j)-\int_0^{x_i}f''(u)\,du$$

(2.3) $$A_0(t)=1, \quad A_1(t)=t, \quad A_2(t)=\frac{1}{2}t^2-\frac{1}{6}t^3, \quad A_3(t)=\frac{1}{6}t^3$$

and $t=(x-x_i)/h$.

The coefficients s_i and s'_i in (2.2) are given by the recurrence formulae:

$$s'_i=s'_{i-1}+\frac{h}{2}(f''_{i-1}+f''_i),$$

(2.4) $$s_i=s_{i-1}+h\,s'_{i-1}+\frac{h^2}{6}(2f''_{i-1}+f''_i),$$

$$s_0=f_0, \quad s'_0=f'_0, \quad (i=1,2,\dots,N).$$

Proof. If $P_3(t)$ is a cubic polynomial in $[0,1]$, then it can be written as

$$P_3(t)=P_3(0)A_0(t)+P'_3(0)A_1(t)+P''_3(0)A_2(t)+P''_3(1)A_3(t).$$

To determine A_0, A_1, A_2 and A_3 we write the equality for $P_3(t)\equiv 1$, t, t^2 and t^3. We obtain the linear system

$$\begin{aligned} 1&=A_0(t)\\ t&=A_1(t)\\ t^2&=2A_2(t)+2A_3(t)\\ t^3&=6A_3(t) \end{aligned}$$

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Now for a fixed $i\in\{0,1,\dots,N-1\}$, set $x=x_i+\text{th}$, $0\leqq t\leqq 1$. In $[x_i, x_{i+1}]$ the cubic spline $s(x)$ which satisfies (2.1) is

$$s(x)=s_iA_0(t)+hs'_iA_1(t)+h^2f''_iA_2(t)+h^2f''_{i+1}A_3(t).$$

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(3.1) $$|s'_i-f'_i|\leqq\frac{h^2}{12}\|f^{(4)}\|$$

Proof. We have from (2.4)

$$s'_i=s'_0+\frac{h}{2}(f''_0+f''_i+2\sum_{j=1}^{i-1}f''_j).$$

Thus

(3.2) $$s'_i-f'_i=s'_0-f'_0+\frac{h}{2}(f''_0+f''_i+2\sum_{j=1}^{i-1}f''_j)-\int_0^{x_i}f''(u)\,du$$

But $s'_0=f'_0$, therefore, using the error term of the classical trapezoidal rule, (3.2) leads to

$$|s'_i-f'_i|\leq \frac{h^2}{12}x_i\|f^{(4)}\|\leq \frac{h^2}{12}\|f^{(4)}\|.$$

This completes the proof.

Lemma 2. *Let $s(x)$ be the cubic spline defined in (2.2) and (2.4). If $f\in C^4[0,1]$, then for* $i=1,2,\dots,N$

$$|s_i-f_i|\leq \left(\frac{h^2}{12}+\frac{h^3}{24}\right)\|f^{(4)}\|. \tag{3.3}$$

Proof. Using (2.4) we have

$$s_i-f_i=s_{i-1}-f_{i-1}+hs'_{i-1}+\frac{h^2}{6}(2f''_{i-1}+f''_i)+f_{i-1}-f_i.$$

Expanding the right hand side about x_{i-1} using Taylor's expansion of order 4 with integral remainder and the Mean Value Theorem for integrals, we get

$$s_i-f_i=s_{i-1}-f_{i-1}+h(s'_{i-1}-f'_{i-1})+\frac{h^4}{24}f^{(4)}(\xi_i),$$

where $\xi_i\in[x_{i-1}, x_i]$. It follows, using (3.1), that

$$|s_i-f_i|\leq|s_{i-1}-f_{i-1}|+\frac{h^3}{12}\|f^{(4)}\|+\frac{h^4}{24}\|f^{(4)}\|$$

which leads to (3.3)

Theorem 2. *Let $s(x)$ be the cubic spline defined in (2.2) and (2.4). If $f\in C^4$ $[0,1]$ then for any $x\in[0,1]$.*

$$\begin{aligned}
&|s'''(x)-f'''(x)|\leq\frac{1}{2}h\|f^{(4)}\|,\\
&|s''(x)-f'(x)|\leq\frac{1}{8}h^2\|f^{(4)}\|,\\
&|s'(x)-f'(x)|\leq\left(\frac{1}{12}h^2+\frac{5}{12}h^3\right)\|f^{(4)}\|,\\
&|s(x)-f(x)|\leq\left(\frac{1}{12}h^2+\frac{1}{8}h^3+\frac{1}{8}h^4\right)\|f^{(4)}\|.
\end{aligned}\tag{3.4}$$

Proof. Differentiating both sides of (2.2) with respect to x ($x=x_i+\mathrm{th}$) we get

$$s'(x)=s'_i+\left(t-\frac{1}{2}t^2\right)hf''_i+\frac{1}{2}t^2hf''_{i+1}, \tag{3.5}$$

$$s''(x)=(1-t)f''_i+tf''_{i+1}, \tag{3.6}$$

$$s'''(x)=\frac{1}{h}(f''_{i+1}-f''_i). \tag{3.7}$$

Subtracting $f'''(x)$ from both sides of (3.7) and expanding the right hand side about x_i by Taylor's expansion of order 4 with integral remainder and using the Mean Value Theorem for integrals, we get

$$s'''(x)-f'''(x)=-\frac{h}{2}t^2f^{(4)}(\alpha_i)+\frac{h}{2}(1-t)^2f^{(4)}(\beta_i),$$

where α_i, $\beta_i \in [x_{i-1}, x_i]$. Therefore (3. 4. 1) is satisfied. (3. 4. 2) follows from the classical error of the linear interpolation since $s''(x)$ is a linear interpolation for f'' in $[x_{i-1}, x_i]$. To show (3.4.3), we subtract $f'(x)$ from both sides of (3.5) and expand using Taylor's expansion of order 4 about x_i. We get

$$s'(x)-f'(x)=s_i'-f_i'+\frac{h^3t^2}{4}f^{(4)}(\alpha_i)-\frac{h^3t^3}{6}f^{(4)}(\beta_i)$$

$\{\alpha_i, \beta_i \in [x_{i-1}, x_i]\}$ which, with (3.1) gives the result. Finally, in a similar manner, we get after expansion

$$s(x)-f(x)=s_i-f_i+th(s_i'-f_i')+\frac{t^3h^4}{12}f^{(4)}(\alpha_i)-\frac{t^4h^4}{24}f^{(4)}(\beta_i)$$

α_i, $\beta_i \in [x_{i-1}, x_i]$. This, using (3.1) and (3.3) leads to (3.4.4). This completes the proof.

4. The Periodic Case (Existence and Uniqueness). Using the same notation as the previous case, we prove the following theorem.

Theorem 3. *Given the real numbers* f_i'' $(i=0,1,\dots, N)$, f_0 *and* f_N *such that* $f_0=f_N$, *there exists a unique periodic cubic spline* $s \in S_{N,3}^{(2)}$ *such that*

$$(4.1)\qquad \begin{aligned} &s_i''=f_i''\ (i=0,1,\dots, N),\\ &s_0=s_N=f_0=f_N \text{ given.}\end{aligned}$$

The cubic spline that satisfies (4.1) *in* $[x_i, x_{i+1}]$ *is*

$$(4.2)\qquad s(x)=s_iA_0(t)+hs_i'A_1(t)+h^2f_i''A_2(t)+h^2f_{i+1}''A_3(t),$$

where A_0, A_1, A_2 *and* A_3 *are the same given in (2.3) for the nonperiodic case. The coefficients* s_i, s_i' *in (4.2) are given by the recurrence formulae*

$$(4.3)\qquad \begin{aligned} &s_0'=h^2\sum_{i=1}^{N-1}(i-N)f_i''-\frac{h^2}{6}[f_N''+(3N-1)f_0''],\\ &s_i'=s_{i-1}'+\frac{h}{2}(f_{i-1}''+f_i''),\quad (i=1, 2,\dots, N),\\ &s_i=s_{i-1}+hs_{i-1}'+\frac{h^2}{6}(2f_{i-1}''+f_i''),\ s_0=f_0,\quad (i=1, 2,\dots, N).\end{aligned}$$

Proof. (4.2), (4.3.2) and (4.3.3) are the same as (2.2) and (2.4) except that here s_0' is unknown. To compute it we observe, from (4.3.3), that

$$s_i=s_0+hs_0'+\frac{h^2}{6}(2f_0''+f_1''),$$

$$s_2=s_1+hs_1'+\frac{h^2}{6}(2f_1''+f_2''),$$

$$\vdots$$

$$s_N=s_{N-1}+hs_{N-1}^1+\frac{h^2}{6}(2f_{N-1}''+f_N'').$$

Adding both sides and using the periodicity $s_N = s_0$, we obtain

$$(4.4)\qquad s'_0 + s'_1 + \cdots + s'_{N-1} = \frac{-h}{6}\left(2f''_0 + f''_N + 3\sum_{j=1}^{N-1} f''_j\right).$$

This equation, together with the N equations of (4.3.2), forms a linear system of $(N+1)$ equations with the $(N+1)$ unknown $s'_0, s'_1, \ldots, s'_N$. This system is

$$(4, 5)\qquad \begin{bmatrix} -1 & 1 & 0 & \cdots & \cdots & 0 \\ 0 & -1 & 1 & 0 & \cdots & 0 \\ \vdots & \ddots & \ddots & \ddots & \ddots & \vdots \\ \vdots & & \ddots & \ddots & \ddots & 0 \\ 0 & \cdots & \cdots & 0 & -1 & 1 \\ 1 & 1 & \cdots & \cdots & 1 & 0 \end{bmatrix} \begin{bmatrix} s'_0 \\ s'_1 \\ \vdots \\ \vdots \\ s'_{N-1} \\ s'_N \end{bmatrix} = \begin{bmatrix} b_0 \\ b_1 \\ \vdots \\ \vdots \\ b_{N-1} \\ b_N \end{bmatrix}$$

Fig. 1

where $b_i = \frac{h}{2}(f''_1 + f''_{i+1})$, $i = 0,1, \ldots, N-1$, and b_N is the right hand side of (4.4). The coefficient matrix of the above linear system say A, is nonsingular with inverse equal to

$$A^{-1} = \frac{1}{N} \begin{bmatrix} -(N-1) & -(N-2) & -(N-3) & \cdots & -1 & 0 & 1 \\ 1 & -(N-2) & -(N-3) & \cdots & -1 & 0 & 1 \\ 1 & 2 & -(N-3) & \cdots & -1 & 0 & 1 \\ 1 & 2 & 3 & \ddots & \vdots & \vdots & \vdots \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ 1 & 2 & 3 & & -1 & 0 & 1 \\ 1 & 2 & 3 & \cdots & N-1 & 0 & 1 \\ 1 & 2 & 3 & \cdots & N-1 & N & 1 \end{bmatrix}$$

Fig. 2

Table 2. Maximum absolute errors for Example 2.
$f(x) = -x + \sin \frac{\pi}{2} x$ in [0,1] (nonperiodic case) for various values of h

Maximum error bound for	Step size $h = \frac{1}{N}$					
	0.1	0.05	0.025	0.02	0.0125	0.01
$\|s-f\|$	1.2×10^{-3}	$2{,}9\times10^{-4}$	7.3×10^{-5}	4.7×10^{-5}	1.8×10^{-5}	1.2×10^{-5}
$\|s'-f'\|$	3.2×10^{-3}	8.1×10^{-4}	2.0×10^{-4}	1.3×10^{-4}	5.0×10^{-5}	3.2×10^{-5}
$\|s''-f''\|$	7.6×10^{-3}	1.9×10^{-3}	4.8×10^{-4}	3.0×10^{-4}	1.2×10^{-4}	7.6×10^{-5}
$s'''-f'''\|$	3.0×10^{-1}	1.5×10^{-1}	7.6×10^{-2}	6.1×10^{-2}	3.8×10^{-2}	3.0×10^{-2}

riodic cubic spline of Section 2. given by (2.2) and (2.4). We notice again the agreement of these numerical results with the corresponding error bounds (3.4).

Example 3. $y'' = 12x^2 - 6x$ in $[0,1]$,

$$y(0) = y(1) = 0.$$

This example has the exact periodic solution $y = f(x) = x^3(x-1)$. The numerical results in Table 3 gives the maximum absolute errors for s-f and its first three derivatives at any point in $[0,1]$ for the values of $h = \frac{1}{N}$, (N= 10, 20, 40, 50, 80, 100). s here is the direct periodic cubic spline of Section 4, defined by (4.2) and (4.3). We can see how the numerical results agree with the corresponding theoretical ones of (5.1). Again the error bounds in (5.1) are best possible for $\| s'' - f'' \|$ only.

Table 3. Maximum absolute errors for Example 3.
$f(x) = x^3(x-1)$ in [0,1] for various values of h

Maximum error bound of	Step size $h = \frac{1}{N}$					
	0.1	0.05	0.025	0.02	0.0125	0.01
$\|s-f\|$	2.5×10^{-3}	6.2×10^{-4}	1.6×10^{-4}	1.0×10^{-4}	3.9×10^{-5}	2.5×10^{-5}
$\|s'-f'\|$	1.0×10^{-2}	2.5×10^{-3}	6.2×10^{-4}	4.0×10^{-4}	1.6×10^{-4}	1.0×10^{-4}
$\|s''-f''\|$	3.0×10^{-2}	7.5×10^{-3}	1.9×10^{-3}	1.2×10^{-3}	4.7×10^{-4}	3.0×10^{-4}
$\|s'''-f'''\|$	1.2	6.0×10^{-1}	3.0×10^{-1}	2.4×10^{-1}	1.5×10^{-1}	1.2×10^{-1}

Example 4. $y'' = -\frac{\pi^2}{4} \sin \frac{\pi}{2} x$ in $[0,1]$,

$$y(0) = y(1) = 0.$$

This example has the exact periodic solution $y=f(x)=-x+\sin\frac{\pi}{2}x$. Table 4 gives the numerical results for this example. On the one hand, we notice the agreement of these numerical results with the corresponding error bounds of (5.1). On the other hand, we observe that the direct periodic cubic spline, (4.2) and (4.3), and the direct nonperiodic cubic spline (2.2) and (2.4) give the same approximation for f'' and f'''. (This is always true since $s''(x)$ and $s'''(x)$, computed from (2.2) or (4.2), are identical.) Also the direct periodic cubic spline gave slightly better results than the nonperiodic cubic spline for the same function $f(x)=-x+\sin\frac{\pi}{2}x$.

Table 4. Maximum absolute errors for Example 4.
$f(x)=-x+\sin\frac{\pi}{2}x$ in [0,1] (periodic case) for various values of h

Maximum error bound of	Step size $h=\frac{1}{N}$					
	0.1	0.05	0.025	0.02	0.0125	0.01
$\|s-f\|$	4.3×10^{-4}	1.1×10^{-4}	2.7×10^{-5}	1.7×10^{-5}	6.8×10^{-6}	4.3×10^{-6}
$\|s'-f'\|$	2.1×10^{-3}	5.1×10^{-4}	1.3×10^{-4}	8.2×10^{-5}	3.2×10^{-5}	2.1×10^{-5}
$\|s''-f''\|$	7.0×10^{-3}	1.9×10^{-3}	4.8×10^{-4}	3.0×10^{-4}	1.2×10^{-4}	7.6×10^{-5}
$\|s'''-f'''\|$	3.0×10^{-1}	1.5×10^{-1}	7.6×10^{-2}	6.1×01^{-2}	3.8×10^{-2}	3.0×10^{-2}

7. Conclusion. We have studied the existence and uniqueness of a direct nonperiodic (up to initial conditions) cubic spline and of a direct periodic (up to boundary conditions) cubic spline that both fit the second derivatives of a given function at mesh points. Error bounds for the function and its first three derivatives are derived for both cases which, together with the numerical results, showed the proposed splines to be efficient.

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